Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2023 – 10:11 AM EDT

PDB ID	:	3ZNJ
Title	:	Crystal structure of unliganded ClcF from R.opacus 1CP in crystal form 1.
Authors	:	Roth, C.; Groening, J.A.D.; Kaschabek, S.R.; Schloemann, M.; Straeter, N.
Deposited on	:	2013-02-14
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

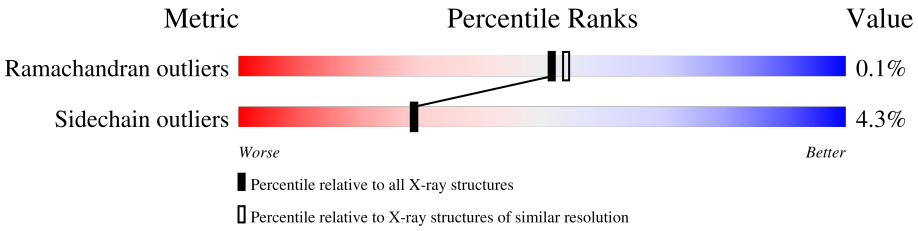
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1	94	95% 5%
1	2	94	91% 7% •
1	3	94	94% • •
1	4	94	98% •
1	5	94	93% 5% •
1	6	94	96% •
1	7	94	97% • •
1	8	94	94% 5% •
1	9	94	91% 5% •

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Mol	Chain	Length	Quality of chain
1	A	94	97%
1	B	94	94% 6%
1	C	94	99%
1	D	94	97%
1	E	94	96%
1	F	94	90% 10%
1	G	94	99%
1	H	94	98%
1	I	94	100%
1	J	94	96%
1	K	94	99%
1	L	94	96%
1	M	94	97%
1	N	94	98%
1	O	94	97%
1	P	94	96%
1	R	94	99%
1	S	94	99%
1	T	94	97%
1	U	94	95% 5%
1	V	94	95% 5%
1	W	94	95% 5%
1	X	94	94% 6%
1	Y	94	91% 5%
1	Z	94	97%

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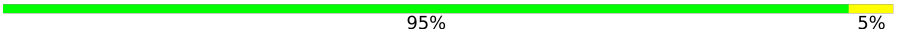
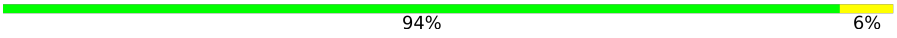
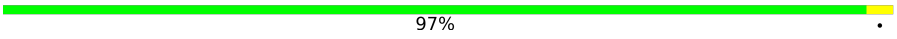
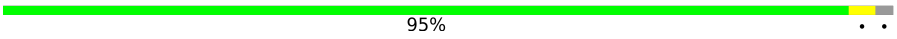
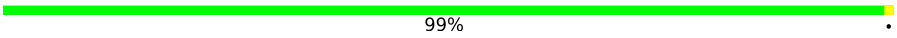
Mol	Chain	Length	Quality of chain
1	a	94	
1	b	94	
1	c	94	
1	d	94	
1	e	94	
1	f	94	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 66372 atoms, of which 31697 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 5-CHLOROMUCONOLACTONE DEHALOGENASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	2	93	Total	C	H	N	O	S	0	0	0
			1562	500	779	142	139	2			
1	3	92	Total	C	H	N	O	S	0	0	0
			1544	494	768	141	139	2			
1	4	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	5	92	Total	C	H	N	O	S	0	0	0
			1540	494	766	140	138	2			
1	6	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	7	92	Total	C	H	N	O	S	0	0	0
			1540	494	766	140	138	2			
1	8	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	9	91	Total	C	H	N	O	S	0	0	0
			1523	490	759	136	136	2			
1	A	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	B	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	C	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	D	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	E	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	F	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	G	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	H	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	I	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	J	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	K	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	L	94	Total	C	H	N	O	S	0	1	0
			1587	508	789	143	145	2			
1	M	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	N	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	O	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	P	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	R	94	Total	C	H	N	O	S	0	1	0
			1591	509	794	143	143	2			
1	S	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	T	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	U	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	V	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	W	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	X	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	Y	91	Total	C	H	N	O	S	0	1	0
			1545	496	769	139	139	2			
1	Z	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	a	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	b	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	c	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	d	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	e	92	Total	C	H	N	O	S	0	0	0
			1540	494	766	140	138	2			
1	f	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1	1	Total	Cl	0	0
			1	1		
2	2	1	Total	Cl	0	0
			1	1		
2	3	1	Total	Cl	0	0
			1	1		
2	4	1	Total	Cl	0	0
			1	1		
2	5	1	Total	Cl	0	0
			1	1		
2	6	1	Total	Cl	0	0
			1	1		
2	7	1	Total	Cl	0	0
			1	1		
2	8	1	Total	Cl	0	0
			1	1		
2	9	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		
2	C	1	Total	Cl	0	0
			1	1		
2	D	1	Total	Cl	0	0
			1	1		
2	E	1	Total	Cl	0	0
			1	1		
2	F	1	Total	Cl	0	0
			1	1		
2	G	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total Cl 1 1	0	0
2	I	1	Total Cl 1 1	0	0
2	J	1	Total Cl 1 1	0	0
2	K	1	Total Cl 1 1	0	0
2	L	1	Total Cl 1 1	0	0
2	M	1	Total Cl 1 1	0	0
2	N	1	Total Cl 1 1	0	0
2	O	1	Total Cl 1 1	0	0
2	P	1	Total Cl 1 1	0	0
2	R	1	Total Cl 1 1	0	0
2	S	1	Total Cl 1 1	0	0
2	T	1	Total Cl 1 1	0	0
2	U	1	Total Cl 1 1	0	0
2	V	1	Total Cl 1 1	0	0
2	W	1	Total Cl 1 1	0	0
2	X	1	Total Cl 1 1	0	0
2	Y	1	Total Cl 1 1	0	0
2	Z	1	Total Cl 1 1	0	0
2	a	1	Total Cl 1 1	0	0
2	b	1	Total Cl 1 1	0	0
2	c	1	Total Cl 1 1	0	0

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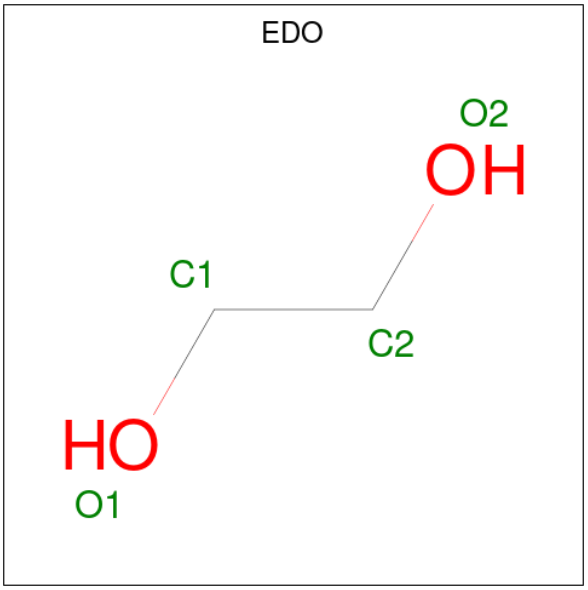
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	d	1	Total Cl 1 1	0	0
2	e	1	Total Cl 1 1	0	0
2	f	1	Total Cl 1 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	1	1	Total C H O 10 2 6 2	0	0
3	1	1	Total C H O 10 2 6 2	0	0
3	2	1	Total C H O 10 2 6 2	0	0
3	2	1	Total C H O 10 2 6 2	0	0
3	3	1	Total C H O 10 2 6 2	0	0
3	3	1	Total C H O 10 2 6 2	0	0
3	4	1	Total C H O 10 2 6 2	0	0
3	4	1	Total C H O 10 2 6 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	5	1	Total	C	H	O	0	0
			10	2	6	2		
3	5	1	Total	C	H	O	0	0
			10	2	6	2		
3	6	1	Total	C	H	O	0	0
			10	2	6	2		
3	6	1	Total	C	H	O	0	0
			10	2	6	2		
3	7	1	Total	C	H	O	0	0
			10	2	6	2		
3	7	1	Total	C	H	O	0	0
			10	2	6	2		
3	8	1	Total	C	H	O	0	0
			10	2	6	2		
3	8	1	Total	C	H	O	0	0
			10	2	6	2		
3	9	1	Total	C	H	O	0	0
			10	2	6	2		
3	9	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	D	1	Total	C	H	O	0	0
			10	2	6	2		
3	D	1	Total	C	H	O	0	0
			10	2	6	2		
3	E	1	Total	C	H	O	0	0
			10	2	6	2		
3	E	1	Total	C	H	O	0	0
			10	2	6	2		
3	F	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	F	1	Total	C	H	O	0	0
			10	2	6	2		
3	G	1	Total	C	H	O	0	0
			10	2	6	2		
3	G	1	Total	C	H	O	0	0
			10	2	6	2		
3	H	1	Total	C	H	O	0	0
			10	2	6	2		
3	H	1	Total	C	H	O	0	0
			10	2	6	2		
3	I	1	Total	C	H	O	0	0
			10	2	6	2		
3	I	1	Total	C	H	O	0	0
			10	2	6	2		
3	J	1	Total	C	H	O	0	0
			10	2	6	2		
3	J	1	Total	C	H	O	0	0
			10	2	6	2		
3	K	1	Total	C	H	O	0	0
			10	2	6	2		
3	K	1	Total	C	H	O	0	0
			10	2	6	2		
3	L	1	Total	C	H	O	0	0
			10	2	6	2		
3	L	1	Total	C	H	O	0	0
			10	2	6	2		
3	M	1	Total	C	H	O	0	0
			10	2	6	2		
3	M	1	Total	C	H	O	0	0
			10	2	6	2		
3	N	1	Total	C	H	O	0	0
			10	2	6	2		
3	N	1	Total	C	H	O	0	0
			10	2	6	2		
3	O	1	Total	C	H	O	0	0
			10	2	6	2		
3	O	1	Total	C	H	O	0	0
			10	2	6	2		
3	P	1	Total	C	H	O	0	0
			10	2	6	2		
3	P	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	R	1	Total	C	H	O	0	0
			10	2	6	2		
3	R	1	Total	C	H	O	0	0
			10	2	6	2		
3	S	1	Total	C	H	O	0	0
			10	2	6	2		
3	S	1	Total	C	H	O	0	0
			10	2	6	2		
3	T	1	Total	C	H	O	0	0
			10	2	6	2		
3	T	1	Total	C	H	O	0	0
			10	2	6	2		
3	U	1	Total	C	H	O	0	0
			10	2	6	2		
3	V	1	Total	C	H	O	0	0
			10	2	6	2		
3	V	1	Total	C	H	O	0	0
			10	2	6	2		
3	W	1	Total	C	H	O	0	0
			10	2	6	2		
3	W	1	Total	C	H	O	0	0
			10	2	6	2		
3	X	1	Total	C	H	O	0	0
			10	2	6	2		
3	X	1	Total	C	H	O	0	0
			10	2	6	2		
3	Y	1	Total	C	H	O	0	0
			10	2	6	2		
3	Y	1	Total	C	H	O	0	0
			10	2	6	2		
3	Z	1	Total	C	H	O	0	0
			10	2	6	2		
3	a	1	Total	C	H	O	0	0
			10	2	6	2		
3	a	1	Total	C	H	O	0	0
			10	2	6	2		
3	b	1	Total	C	H	O	0	0
			10	2	6	2		
3	b	1	Total	C	H	O	0	0
			10	2	6	2		
3	c	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	c	1	Total	C	H	O	0	0
			10	2	6	2		
3	d	1	Total	C	H	O	0	0
			10	2	6	2		
3	d	1	Total	C	H	O	0	0
			10	2	6	2		
3	e	1	Total	C	H	O	0	0
			10	2	6	2		
3	e	1	Total	C	H	O	0	0
			10	2	6	2		
3	f	1	Total	C	H	O	0	0
			10	2	6	2		
3	f	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1	57	Total	O	0	0
			57	57		
4	2	59	Total	O	0	0
			59	59		
4	3	68	Total	O	0	0
			68	68		
4	4	38	Total	O	0	0
			38	38		
4	5	47	Total	O	0	0
			47	47		
4	6	46	Total	O	0	0
			46	46		
4	7	41	Total	O	0	0
			41	41		
4	8	56	Total	O	0	0
			56	56		
4	9	50	Total	O	0	0
			50	50		
4	A	155	Total	O	0	0
			155	155		
4	B	143	Total	O	0	0
			143	143		
4	C	169	Total	O	0	0
			169	169		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	147	Total O 147 147	0	0
4	E	161	Total O 161 161	0	0
4	F	122	Total O 122 122	0	0
4	G	138	Total O 138 138	0	0
4	H	93	Total O 93 93	0	0
4	I	75	Total O 75 75	0	0
4	J	90	Total O 90 90	0	0
4	K	103	Total O 103 103	0	0
4	L	87	Total O 87 87	0	0
4	M	84	Total O 84 84	0	0
4	N	78	Total O 78 78	0	0
4	O	64	Total O 64 64	0	0
4	P	67	Total O 67 67	0	0
4	R	95	Total O 95 95	0	0
4	S	88	Total O 88 88	0	0
4	T	82	Total O 82 82	0	0
4	U	54	Total O 54 54	0	0
4	V	46	Total O 46 46	0	0
4	W	37	Total O 37 37	0	0
4	X	42	Total O 42 42	0	0
4	Y	29	Total O 29 29	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Z	44	Total O 44 44	0	0

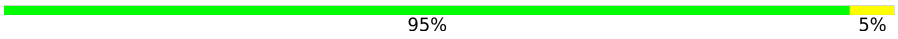
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

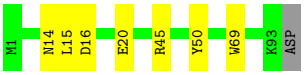
• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain 1:



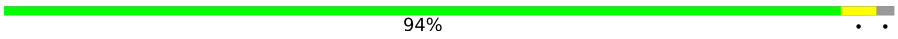
• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain 2:



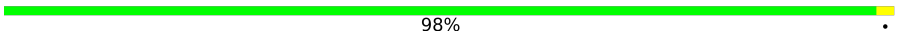
• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain 3:



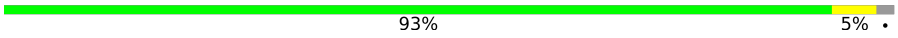
• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain 4:



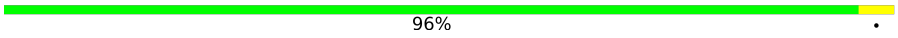
• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain 5:



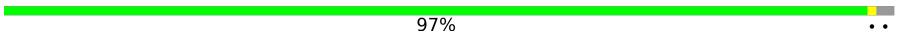
• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

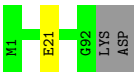
Chain 6:



• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

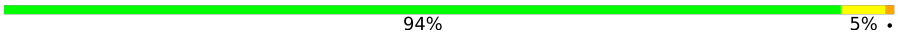
Chain 7:

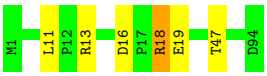




• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

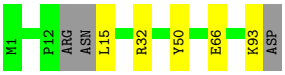
Chain 8:





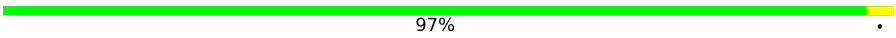
• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain 9:



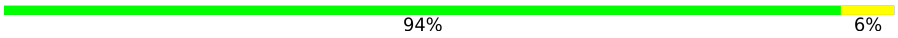
• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

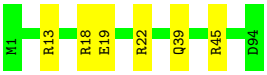
Chain A:



• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

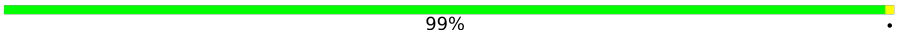
Chain B:





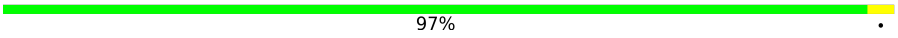
• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

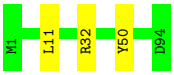
Chain C:



• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

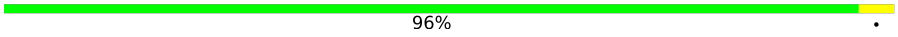
Chain D:

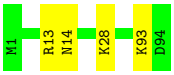




• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain E:



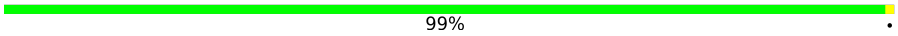


• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain F:

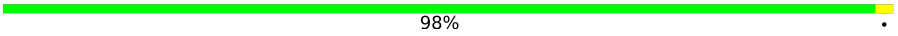
• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain G:



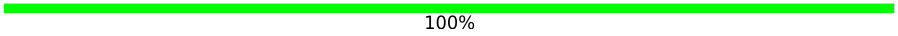
• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain H:



• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

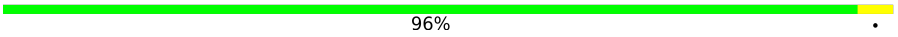
Chain I:



There are no outlier residues recorded for this chain.

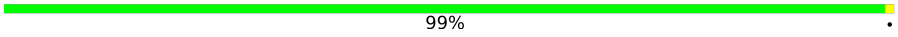
• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain J:



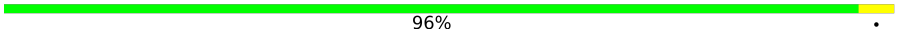
• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain K:



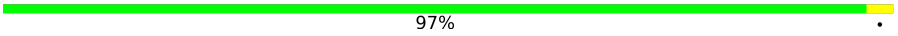
• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

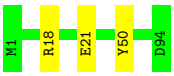
Chain L:



• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

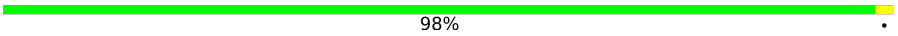
Chain M:





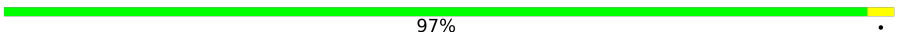
• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain N:



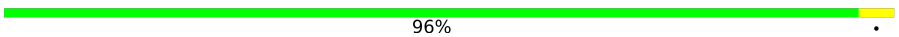
• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain O:



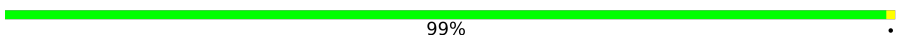
• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain P:



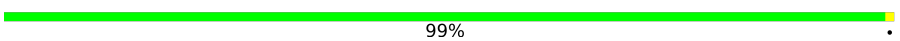
• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain R:



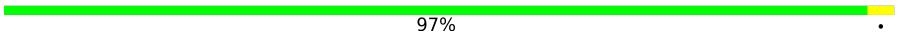
• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

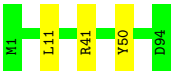
Chain S:



• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

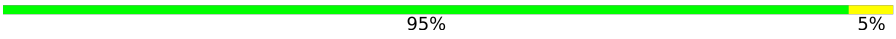
Chain T:





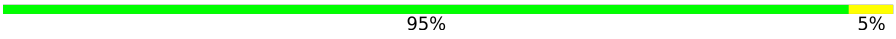
• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain U:



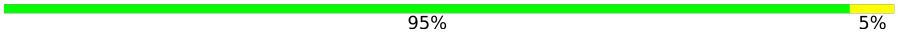
• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

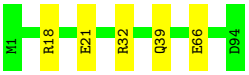
Chain V:



• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

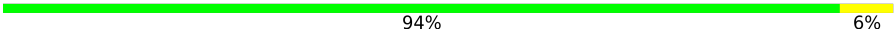
Chain W:

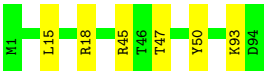




• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

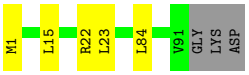
Chain X:





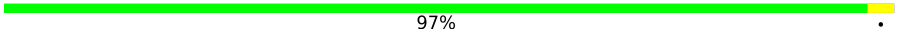
• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

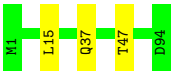
Chain Y:



• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

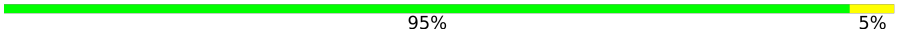
Chain Z:





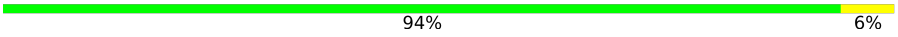
• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain a:



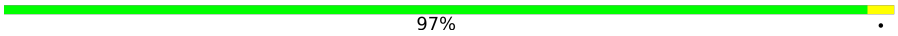
• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

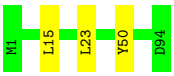
Chain b:



• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

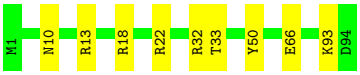
Chain c:





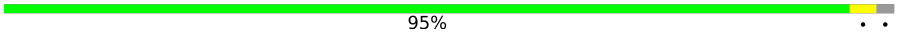
• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

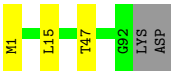
Chain d:



• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

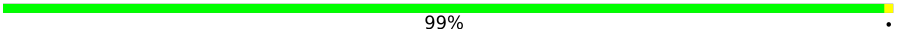
Chain e:





• Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain f:



4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	151.14Å 79.43Å 198.97Å 90.00° 93.41° 90.00°	Depositor
Resolution (Å)	19.90 – 2.10	Depositor
% Data completeness (in resolution range)	95.3 (19.90-2.10)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.33 (at 2.09Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: DEV_1172)	Depositor
R, R_{free}	0.164 , 0.224	Depositor
Wilson B-factor (Å^2)	25.7	Xtriage
Anisotropy	0.187	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	66372	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.69% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	1	0.23	0/814	0.44	0/1103
1	2	0.23	0/805	0.44	0/1092
1	3	0.23	0/797	0.45	0/1077
1	4	0.24	0/814	0.44	0/1103
1	5	0.23	0/796	0.42	0/1081
1	6	0.23	0/814	0.44	0/1103
1	7	0.23	0/796	0.45	0/1081
1	8	0.24	0/814	0.52	1/1103 (0.1%)
1	9	0.22	0/785	0.44	0/1064
1	A	0.23	0/814	0.44	0/1103
1	B	0.24	0/814	0.43	0/1103
1	C	0.23	0/814	0.43	0/1103
1	D	0.24	0/814	0.45	0/1103
1	E	0.24	0/814	0.44	0/1103
1	F	0.24	0/814	0.45	0/1103
1	G	0.24	0/814	0.43	0/1103
1	H	0.24	0/814	0.47	0/1103
1	I	0.24	0/814	0.44	0/1103
1	J	0.24	0/814	0.45	0/1103
1	K	0.23	0/814	0.45	0/1103
1	L	0.24	0/823	0.45	0/1115
1	M	0.23	0/814	0.44	0/1103
1	N	0.23	0/814	0.45	0/1103
1	O	0.24	0/814	0.45	0/1103
1	P	0.24	0/814	0.45	0/1103
1	R	0.24	0/822	0.44	0/1114
1	S	0.24	0/814	0.44	0/1103
1	T	0.24	0/814	0.45	0/1103
1	U	0.24	0/814	0.47	0/1103
1	V	0.23	0/814	0.44	0/1103
1	W	0.24	0/814	0.47	0/1103
1	X	0.23	0/814	0.44	0/1103

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	Y	0.24	0/801	0.44	0/1088
1	Z	0.24	0/814	0.45	0/1103
1	a	0.23	0/814	0.45	0/1103
1	b	0.23	0/814	0.44	0/1103
1	c	0.23	0/814	0.43	0/1103
1	d	0.24	0/814	0.45	0/1103
1	e	0.24	0/796	0.49	0/1081
1	f	0.25	0/814	0.45	0/1103
All	All	0.24	0/32455	0.45	1/43986 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	8	18	ARG	NE-CZ-NH1	7.32	123.96	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1	92/94 (98%)	89 (97%)	2 (2%)	1 (1%)	14 9
1	2	91/94 (97%)	89 (98%)	2 (2%)	0	100 100
1	3	88/94 (94%)	86 (98%)	2 (2%)	0	100 100
1	4	92/94 (98%)	90 (98%)	2 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5	90/94 (96%)	88 (98%)	2 (2%)	0	100	100
1	6	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
1	7	90/94 (96%)	86 (96%)	4 (4%)	0	100	100
1	8	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
1	9	87/94 (93%)	85 (98%)	2 (2%)	0	100	100
1	A	92/94 (98%)	90 (98%)	1 (1%)	1 (1%)	14	9
1	B	92/94 (98%)	92 (100%)	0	0	100	100
1	C	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
1	D	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
1	E	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
1	F	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
1	G	92/94 (98%)	92 (100%)	0	0	100	100
1	H	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
1	I	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
1	J	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
1	K	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
1	L	93/94 (99%)	93 (100%)	0	0	100	100
1	M	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
1	N	92/94 (98%)	92 (100%)	0	0	100	100
1	O	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
1	P	92/94 (98%)	92 (100%)	0	0	100	100
1	R	93/94 (99%)	93 (100%)	0	0	100	100
1	S	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
1	T	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
1	U	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
1	V	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
1	W	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
1	X	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
1	Y	90/94 (96%)	89 (99%)	1 (1%)	0	100	100
1	Z	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
1	a	92/94 (98%)	91 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	b	92/94 (98%)	92 (100%)	0	0	100	100
1	c	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
1	d	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
1	e	90/94 (96%)	89 (99%)	1 (1%)	0	100	100
1	f	92/94 (98%)	92 (100%)	0	0	100	100
All	All	3664/3760 (97%)	3609 (98%)	53 (1%)	2 (0%)	51	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	17	PRO
1	A	17	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	87/87 (100%)	83 (95%)	4 (5%)	27	26
1	2	86/87 (99%)	79 (92%)	7 (8%)	11	8
1	3	85/87 (98%)	81 (95%)	4 (5%)	26	25
1	4	87/87 (100%)	85 (98%)	2 (2%)	50	55
1	5	85/87 (98%)	80 (94%)	5 (6%)	19	17
1	6	87/87 (100%)	83 (95%)	4 (5%)	27	26
1	7	85/87 (98%)	84 (99%)	1 (1%)	71	77
1	8	87/87 (100%)	81 (93%)	6 (7%)	15	12
1	9	84/87 (97%)	79 (94%)	5 (6%)	19	16
1	A	87/87 (100%)	85 (98%)	2 (2%)	50	55
1	B	87/87 (100%)	81 (93%)	6 (7%)	15	12
1	C	87/87 (100%)	86 (99%)	1 (1%)	73	79
1	D	87/87 (100%)	84 (97%)	3 (3%)	37	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	87/87 (100%)	83 (95%)	4 (5%)	27 26
1	F	87/87 (100%)	78 (90%)	9 (10%)	7 4
1	G	87/87 (100%)	86 (99%)	1 (1%)	73 79
1	H	87/87 (100%)	85 (98%)	2 (2%)	50 55
1	I	87/87 (100%)	87 (100%)	0	100 100
1	J	87/87 (100%)	83 (95%)	4 (5%)	27 26
1	K	87/87 (100%)	86 (99%)	1 (1%)	73 79
1	L	88/87 (101%)	84 (96%)	4 (4%)	27 27
1	M	87/87 (100%)	84 (97%)	3 (3%)	37 39
1	N	87/87 (100%)	85 (98%)	2 (2%)	50 55
1	O	87/87 (100%)	84 (97%)	3 (3%)	37 39
1	P	87/87 (100%)	83 (95%)	4 (5%)	27 26
1	R	88/87 (101%)	87 (99%)	1 (1%)	73 79
1	S	87/87 (100%)	86 (99%)	1 (1%)	73 79
1	T	87/87 (100%)	84 (97%)	3 (3%)	37 39
1	U	87/87 (100%)	82 (94%)	5 (6%)	20 18
1	V	87/87 (100%)	82 (94%)	5 (6%)	20 18
1	W	87/87 (100%)	82 (94%)	5 (6%)	20 18
1	X	87/87 (100%)	81 (93%)	6 (7%)	15 12
1	Y	86/87 (99%)	81 (94%)	5 (6%)	20 17
1	Z	87/87 (100%)	84 (97%)	3 (3%)	37 39
1	a	87/87 (100%)	82 (94%)	5 (6%)	20 18
1	b	87/87 (100%)	81 (93%)	6 (7%)	15 12
1	c	87/87 (100%)	84 (97%)	3 (3%)	37 39
1	d	87/87 (100%)	78 (90%)	9 (10%)	7 4
1	e	85/87 (98%)	82 (96%)	3 (4%)	36 38
1	f	87/87 (100%)	86 (99%)	1 (1%)	73 79
All	All	3469/3480 (100%)	3321 (96%)	148 (4%)	29 29

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	11	LEU

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Mol	Chain	Res	Type
1	1	15	LEU
1	1	18	ARG
1	1	93	LYS
1	2	14	ASN
1	2	15	LEU
1	2	16	ASP
1	2	20	GLU
1	2	45	ARG
1	2	50	TYR
1	2	69	TRP
1	3	14	ASN
1	3	19	GLU
1	3	20	GLU
1	3	46	THR
1	4	21	GLU
1	4	23	LEU
1	5	15	LEU
1	5	32	ARG
1	5	41	ARG
1	5	46	THR
1	5	53	ILE
1	6	1	MET
1	6	13	ARG
1	6	50	TYR
1	6	94	ASP
1	7	21	GLU
1	8	11	LEU
1	8	13	ARG
1	8	16	ASP
1	8	18	ARG
1	8	19	GLU
1	8	47	THR
1	9	15	LEU
1	9	32	ARG
1	9	50	TYR
1	9	66	GLU
1	9	93	LYS
1	A	19	GLU
1	A	50	TYR
1	B	13	ARG
1	B	18	ARG
1	B	19	GLU

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Mol	Chain	Res	Type
1	B	22	ARG
1	B	39	GLN
1	B	45	ARG
1	C	15	LEU
1	D	11	LEU
1	D	32	ARG
1	D	50	TYR
1	E	13	ARG
1	E	14	ASN
1	E	28	LYS
1	E	93	LYS
1	F	11	LEU
1	F	13	ARG
1	F	15	LEU
1	F	18	ARG
1	F	22	ARG
1	F	30	ARG
1	F	41	ARG
1	F	50	TYR
1	F	93	LYS
1	G	50	TYR
1	H	18	ARG
1	H	23	LEU
1	J	13	ARG
1	J	18	ARG
1	J	23	LEU
1	J	50	TYR
1	K	1	MET
1	L	13	ARG
1	L	23	LEU
1	L	47	THR
1	L	50	TYR
1	M	18	ARG
1	M	21	GLU
1	M	50	TYR
1	N	13	ARG
1	N	50	TYR
1	O	13	ARG
1	O	24	LYS
1	O	47	THR
1	P	22	ARG
1	P	26	SER

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Mol	Chain	Res	Type
1	P	30	ARG
1	P	47	THR
1	R	50	TYR
1	S	50	TYR
1	T	11	LEU
1	T	41	ARG
1	T	50	TYR
1	U	11	LEU
1	U	13	ARG
1	U	15	LEU
1	U	78	THR
1	U	93	LYS
1	V	15	LEU
1	V	21	GLU
1	V	47	THR
1	V	50	TYR
1	V	93	LYS
1	W	18	ARG
1	W	21	GLU
1	W	32	ARG
1	W	39	GLN
1	W	66	GLU
1	X	15	LEU
1	X	18	ARG
1	X	45	ARG
1	X	47	THR
1	X	50	TYR
1	X	93	LYS
1	Y	1	MET
1	Y	15	LEU
1	Y	22	ARG
1	Y	23	LEU
1	Y	84	LEU
1	Z	15	LEU
1	Z	37	GLN
1	Z	47	THR
1	a	10	ASN
1	a	14	ASN
1	a	18	ARG
1	a	22	ARG
1	a	23	LEU
1	b	10	ASN

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Mol	Chain	Res	Type
1	b	11	LEU
1	b	13	ARG
1	b	30	ARG
1	b	32	ARG
1	b	37	GLN
1	c	15	LEU
1	c	23	LEU
1	c	50	TYR
1	d	10	ASN
1	d	13	ARG
1	d	18	ARG
1	d	22	ARG
1	d	32	ARG
1	d	33	THR
1	d	50	TYR
1	d	66	GLU
1	d	93	LYS
1	e	1	MET
1	e	15	LEU
1	e	47	THR
1	f	47	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	61	HIS
1	8	61	HIS
1	C	61	HIS
1	D	61	HIS
1	I	61	HIS
1	J	61	HIS
1	M	61	HIS
1	P	61	HIS
1	S	37	GLN
1	S	39	GLN
1	T	37	GLN
1	V	14	ASN
1	V	61	HIS
1	d	10	ASN
1	f	37	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 118 ligands modelled in this entry, 40 are monoatomic - leaving 78 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	EDO	V	1096	-	3,3,3	0.41	0	2,2,2	0.35	0
3	EDO	8	1096	-	3,3,3	0.43	0	2,2,2	0.58	0
3	EDO	B	1096	-	3,3,3	0.51	0	2,2,2	0.34	0
3	EDO	6	1096	-	3,3,3	0.49	0	2,2,2	0.23	0
3	EDO	H	1096	-	3,3,3	0.57	0	2,2,2	0.40	0
3	EDO	Z	1096	-	3,3,3	0.45	0	2,2,2	0.33	0
3	EDO	S	1096	-	3,3,3	0.44	0	2,2,2	0.32	0
3	EDO	L	1096	-	3,3,3	0.47	0	2,2,2	0.35	0
3	EDO	c	1096	-	3,3,3	0.43	0	2,2,2	0.33	0
3	EDO	P	1096	-	3,3,3	0.46	0	2,2,2	0.31	0
3	EDO	F	1097	-	3,3,3	0.43	0	2,2,2	0.33	0
3	EDO	3	1097	-	3,3,3	0.47	0	2,2,2	0.36	0
3	EDO	X	1097	-	3,3,3	0.46	0	2,2,2	0.28	0
3	EDO	d	1097	-	3,3,3	0.45	0	2,2,2	0.32	0
3	EDO	C	1097	-	3,3,3	0.45	0	2,2,2	0.31	0
3	EDO	9	1095	-	3,3,3	0.43	0	2,2,2	0.62	0
3	EDO	M	1096	-	3,3,3	0.48	0	2,2,2	0.27	0
3	EDO	O	1096	-	3,3,3	0.49	0	2,2,2	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	EDO	e	1094	-	3,3,3	0.48	0	2,2,2	0.46	0
3	EDO	H	1097	-	3,3,3	0.47	0	2,2,2	0.29	0
3	EDO	a	1096	-	3,3,3	0.50	0	2,2,2	0.41	0
3	EDO	W	1096	-	3,3,3	0.43	0	2,2,2	0.35	0
3	EDO	S	1097	-	3,3,3	0.45	0	2,2,2	0.33	0
3	EDO	7	1094	-	3,3,3	0.44	0	2,2,2	0.38	0
3	EDO	3	1096	-	3,3,3	0.44	0	2,2,2	0.24	0
3	EDO	1	1096	-	3,3,3	0.42	0	2,2,2	0.27	0
3	EDO	7	1095	-	3,3,3	0.46	0	2,2,2	0.30	0
3	EDO	V	1097	-	3,3,3	0.46	0	2,2,2	0.30	0
3	EDO	T	1097	-	3,3,3	0.47	0	2,2,2	0.37	0
3	EDO	M	1097	-	3,3,3	0.47	0	2,2,2	0.30	0
3	EDO	P	1097	-	3,3,3	0.44	0	2,2,2	0.26	0
3	EDO	b	1096	-	3,3,3	0.41	0	2,2,2	0.52	0
3	EDO	C	1096	-	3,3,3	0.53	0	2,2,2	0.39	0
3	EDO	N	1097	-	3,3,3	0.45	0	2,2,2	0.33	0
3	EDO	E	1097	-	3,3,3	0.45	0	2,2,2	0.32	0
3	EDO	a	1097	-	3,3,3	0.45	0	2,2,2	0.31	0
3	EDO	O	1097	-	3,3,3	0.47	0	2,2,2	0.30	0
3	EDO	G	1097	-	3,3,3	0.41	0	2,2,2	0.47	0
3	EDO	U	1096	-	3,3,3	0.46	0	2,2,2	0.35	0
3	EDO	b	1097	-	3,3,3	0.47	0	2,2,2	0.26	0
3	EDO	D	1097	-	3,3,3	0.47	0	2,2,2	0.26	0
3	EDO	5	1095	-	3,3,3	0.44	0	2,2,2	0.32	0
3	EDO	8	1097	-	3,3,3	0.45	0	2,2,2	0.32	0
3	EDO	R	1096	-	3,3,3	0.52	0	2,2,2	0.29	0
3	EDO	4	1096	-	3,3,3	0.50	0	2,2,2	0.24	0
3	EDO	R	1097	-	3,3,3	0.46	0	2,2,2	0.35	0
3	EDO	I	1096	-	3,3,3	0.37	0	2,2,2	0.81	0
3	EDO	d	1096	-	3,3,3	0.44	0	2,2,2	0.30	0
3	EDO	A	1097	-	3,3,3	0.47	0	2,2,2	0.24	0
3	EDO	J	1096	-	3,3,3	0.43	0	2,2,2	0.31	0
3	EDO	D	1096	-	3,3,3	0.43	0	2,2,2	0.37	0
3	EDO	T	1096	-	3,3,3	0.45	0	2,2,2	0.32	0
3	EDO	Y	1093	-	3,3,3	0.42	0	2,2,2	0.44	0
3	EDO	5	1094	-	3,3,3	0.46	0	2,2,2	0.33	0
3	EDO	X	1096	-	3,3,3	0.51	0	2,2,2	0.23	0
3	EDO	6	1097	-	3,3,3	0.42	0	2,2,2	0.20	0
3	EDO	4	1097	-	3,3,3	0.42	0	2,2,2	0.31	0
3	EDO	1	1097	-	3,3,3	0.47	0	2,2,2	0.31	0
3	EDO	G	1096	-	3,3,3	0.44	0	2,2,2	0.32	0
3	EDO	J	1097	-	3,3,3	0.47	0	2,2,2	0.27	0
3	EDO	K	1096	-	3,3,3	0.43	0	2,2,2	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	EDO	e	1095	-	3,3,3	0.46	0	2,2,2	0.26	0
3	EDO	f	1097	-	3,3,3	0.47	0	2,2,2	0.25	0
3	EDO	9	1096	-	3,3,3	0.47	0	2,2,2	0.28	0
3	EDO	2	1095	-	3,3,3	0.47	0	2,2,2	0.23	0
3	EDO	F	1096	-	3,3,3	0.49	0	2,2,2	0.35	0
3	EDO	2	1096	-	3,3,3	0.46	0	2,2,2	0.32	0
3	EDO	W	1097	-	3,3,3	0.43	0	2,2,2	0.29	0
3	EDO	A	1096	-	3,3,3	0.43	0	2,2,2	0.34	0
3	EDO	E	1096	-	3,3,3	0.53	0	2,2,2	0.21	0
3	EDO	Y	1094	-	3,3,3	0.47	0	2,2,2	0.26	0
3	EDO	I	1097	-	3,3,3	0.45	0	2,2,2	0.35	0
3	EDO	c	1097	-	3,3,3	0.47	0	2,2,2	0.28	0
3	EDO	B	1097	-	3,3,3	0.44	0	2,2,2	0.33	0
3	EDO	N	1096	-	3,3,3	0.49	0	2,2,2	0.29	0
3	EDO	L	1097	-	3,3,3	0.46	0	2,2,2	0.27	0
3	EDO	K	1097	-	3,3,3	0.47	0	2,2,2	0.26	0
3	EDO	f	1096	-	3,3,3	0.48	0	2,2,2	0.36	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	V	1096	-	-	1/1/1/1	-
3	EDO	8	1096	-	-	0/1/1/1	-
3	EDO	B	1096	-	-	0/1/1/1	-
3	EDO	6	1096	-	-	0/1/1/1	-
3	EDO	H	1096	-	-	0/1/1/1	-
3	EDO	Z	1096	-	-	0/1/1/1	-
3	EDO	S	1096	-	-	0/1/1/1	-
3	EDO	L	1096	-	-	0/1/1/1	-
3	EDO	c	1096	-	-	0/1/1/1	-
3	EDO	P	1096	-	-	0/1/1/1	-
3	EDO	F	1097	-	-	0/1/1/1	-
3	EDO	3	1097	-	-	0/1/1/1	-
3	EDO	X	1097	-	-	0/1/1/1	-
3	EDO	d	1097	-	-	0/1/1/1	-
3	EDO	C	1097	-	-	0/1/1/1	-
3	EDO	9	1095	-	-	1/1/1/1	-
3	EDO	M	1096	-	-	0/1/1/1	-
3	EDO	O	1096	-	-	0/1/1/1	-
3	EDO	e	1094	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	H	1097	-	-	0/1/1/1	-
3	EDO	a	1096	-	-	0/1/1/1	-
3	EDO	W	1096	-	-	0/1/1/1	-
3	EDO	S	1097	-	-	0/1/1/1	-
3	EDO	7	1094	-	-	0/1/1/1	-
3	EDO	3	1096	-	-	0/1/1/1	-
3	EDO	1	1096	-	-	0/1/1/1	-
3	EDO	7	1095	-	-	0/1/1/1	-
3	EDO	V	1097	-	-	1/1/1/1	-
3	EDO	T	1097	-	-	0/1/1/1	-
3	EDO	M	1097	-	-	0/1/1/1	-
3	EDO	P	1097	-	-	0/1/1/1	-
3	EDO	b	1096	-	-	0/1/1/1	-
3	EDO	C	1096	-	-	0/1/1/1	-
3	EDO	N	1097	-	-	0/1/1/1	-
3	EDO	E	1097	-	-	0/1/1/1	-
3	EDO	a	1097	-	-	0/1/1/1	-
3	EDO	O	1097	-	-	1/1/1/1	-
3	EDO	G	1097	-	-	0/1/1/1	-
3	EDO	U	1096	-	-	0/1/1/1	-
3	EDO	b	1097	-	-	0/1/1/1	-
3	EDO	D	1097	-	-	0/1/1/1	-
3	EDO	5	1095	-	-	0/1/1/1	-
3	EDO	8	1097	-	-	0/1/1/1	-
3	EDO	R	1096	-	-	0/1/1/1	-
3	EDO	4	1096	-	-	0/1/1/1	-
3	EDO	R	1097	-	-	0/1/1/1	-
3	EDO	I	1096	-	-	0/1/1/1	-
3	EDO	d	1096	-	-	0/1/1/1	-
3	EDO	A	1097	-	-	0/1/1/1	-
3	EDO	J	1096	-	-	0/1/1/1	-
3	EDO	D	1096	-	-	1/1/1/1	-
3	EDO	T	1096	-	-	0/1/1/1	-
3	EDO	Y	1093	-	-	1/1/1/1	-
3	EDO	5	1094	-	-	0/1/1/1	-
3	EDO	X	1096	-	-	0/1/1/1	-
3	EDO	6	1097	-	-	0/1/1/1	-
3	EDO	4	1097	-	-	1/1/1/1	-
3	EDO	1	1097	-	-	0/1/1/1	-
3	EDO	G	1096	-	-	0/1/1/1	-
3	EDO	J	1097	-	-	0/1/1/1	-
3	EDO	K	1096	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	e	1095	-	-	0/1/1/1	-
3	EDO	f	1097	-	-	0/1/1/1	-
3	EDO	9	1096	-	-	0/1/1/1	-
3	EDO	2	1095	-	-	0/1/1/1	-
3	EDO	F	1096	-	-	1/1/1/1	-
3	EDO	2	1096	-	-	0/1/1/1	-
3	EDO	W	1097	-	-	1/1/1/1	-
3	EDO	A	1096	-	-	0/1/1/1	-
3	EDO	E	1096	-	-	0/1/1/1	-
3	EDO	Y	1094	-	-	0/1/1/1	-
3	EDO	I	1097	-	-	0/1/1/1	-
3	EDO	c	1097	-	-	0/1/1/1	-
3	EDO	B	1097	-	-	0/1/1/1	-
3	EDO	N	1096	-	-	0/1/1/1	-
3	EDO	L	1097	-	-	0/1/1/1	-
3	EDO	K	1097	-	-	0/1/1/1	-
3	EDO	f	1096	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	1096	EDO	O1-C1-C2-O2
3	4	1097	EDO	O1-C1-C2-O2
3	W	1097	EDO	O1-C1-C2-O2
3	Y	1093	EDO	O1-C1-C2-O2
3	V	1096	EDO	O1-C1-C2-O2
3	V	1097	EDO	O1-C1-C2-O2
3	O	1097	EDO	O1-C1-C2-O2
3	e	1094	EDO	O1-C1-C2-O2
3	9	1095	EDO	O1-C1-C2-O2
3	D	1096	EDO	O1-C1-C2-O2
3	F	1096	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.